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**U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director***

Abstract

Simple models are constructed which are used to illustrate the interplay between the strong nuclear forces and the Coulomb molecular forces in the description of the resonant dt_μ -fusion process.

Key words: deuterium; meso-molecule; μ -meson; muon catalyzed fusion; muon molecule; t-d-fusion

1. Introduction

The six-body system of muon-catalyzed fusion [1]¹ (five nucleons plus the muon) is so complicated and intricately interwoven that direct visualization of the reaction becomes extremely difficult. In order to make the complicated interplay of the molecular and nuclear physics accessible we will present here models which focus schematically on the fusion dynamics alone, while stripping away many of the details and their associated complications. These details are, in fact, quite essential for an accurate calculation of the fusion rate and the branching ratios into the various final states; for example, in an accurate calculation of the sticking fraction. The models, however, are useful didactic tools, helpful in understanding the complexities of the complete problem.

Let us detail how we arrive at our models in the following steps. (1) We replace all potentials, Coulomb and nuclear, by square wells and barriers. (2) We drop all angular functions, and retain only the remnant of the radial parts, which we further truncate to a one-dimensional problem, that is, to a single coordinate, x . The image of the dt-channel, denoted as channel d, is taken as the region $x > a$; that of the $n\alpha$ -channel, channel n, as $x < -a$, and $x = \pm a$ represent the R-matrix channel radii of the respective channels. (3) We ignore the presence of the muon in the $n\alpha$ -channel, and we represent its interaction with the system in the dt-channel as a weak attractive square well located at $c \leq x \leq c + t = l$. In this way we arrive at our potential shown in figure 1.

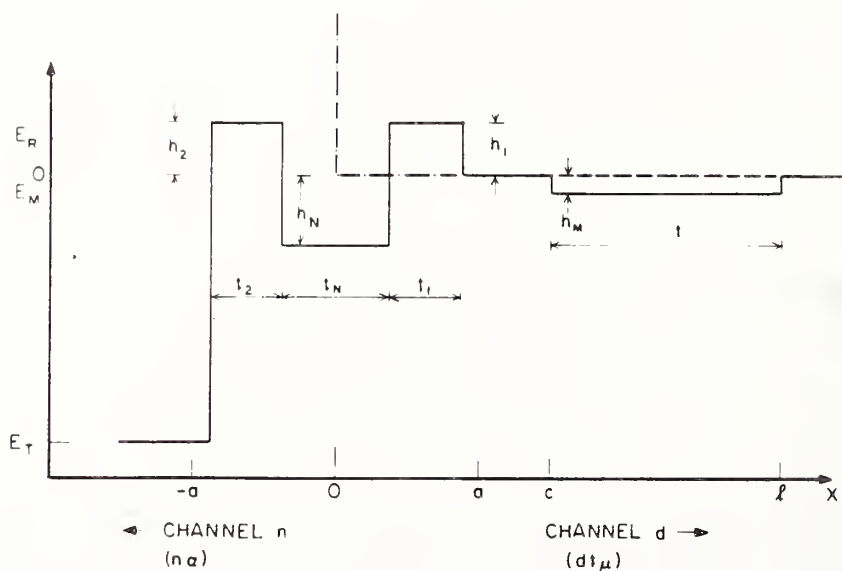


Fig. 1. Potentials for the one dimensional model. See text for explanation.

¹Numbers in square brackets indicate the literature references at the end of this paper.

The full line is the potential of the caricature of the complete $td\mu$ -system. This potential can be adjusted to reproduce the spectrum of the physical system, so that it yields a resonance at E_R (to mimic the 55 keV resonance in ${}^5\text{He}$), while the widths and heights of the barriers, t_1 , h_1 and t_2 , h_2 can be adjusted to reproduce the partial widths. Finally, the parameters of the "muonic potential well", t , h_M and c , can be adjusted to yield a bound state resonance at $E_M \cong -300$ eV and the desired fusion width. For simplicity we shall assume that there exists only a single "molecular bound state," instead of the two $J = 0$ bound states of the real $dt\mu$ -system.

This model, although simple, is still much too complicated to allow for a transparent analytical solution. Let us therefore begin by replacing the finite-range potentials by zero-range (i.e., δ -function) potentials. In this way we will achieve a description which allows a completely explicit solution and thus lends itself to full discussion of the mechanism of the interplay of the different physical components. We do this in section 2. Of course, with this doubly simplified pedagogical model we have moved far enough from actuality that there is no possibility of any quantitative use. Hence we present the discussion of the somewhat more realistic finite-range model in section 3.

2. The Zero-Range Model

In order to solve easily for the nuclear effects we now construct a zero-range nuclear model. Note that on the scale of the μ -molecular ion (~ 500 fm) the nuclear dimensions (~ 2 -3 fm) are indeed small.

The zero-range nuclear model uses the approximation: $k \cot \delta = -1/a$, where a is the Fermi scattering length associated with the nuclear cross section:

$$\sigma = 4\pi \lambda^2 \sin^2 \delta \quad . \quad (2.1)$$

In order to generalize this to two channels, we must first work the in terms of a Hamiltonian:

$$H \psi(r) = (T + V_{\text{eff}}) \psi(r) = E \psi(r) \quad . \quad (2.2)$$

The effective potential $V_{\text{eff}}(r)$ is to be singular in such a way that

$$\int_{0-}^{0+} V_{\text{eff}} \psi dr = W_0 \psi(0+) \quad . \quad (2.3)$$

Integrating the Hamiltonian equation, (2.2) above, over the same infinitesimal interval we find (we use units such that $\hbar = c = 1$)

$$-\frac{1}{2m} \psi'(0+) + W_0 \psi(0+) = 0 \quad . \quad (2.2a)$$

In other words, the zero-range model is equivalent to imposing the boundary condition

$$\frac{\psi'}{\psi} \Big|_{0+} = 2mW_0 =: -\frac{1}{a} \quad , \quad (2.4)$$

where $\psi(r) \equiv A \sin(kr + \delta)$.

We generalize the singular potential to two channels to obtain:

$$H = \begin{pmatrix} T_d & 0 \\ 0 & T_n \end{pmatrix} + \begin{pmatrix} V_{dd} & V_{dn} \\ V_{nd} & V_{nn} \end{pmatrix} \quad (2.5)$$

and

$$\psi = \begin{pmatrix} A\psi_d \\ B\psi_n \end{pmatrix} \quad . \quad (2.6)$$

Of course, $V_{dn} = V_{nd}$.

Integrating over the interval at the origin, as before, we obtain (we now take into account the different reduced masses in the two channels)

$$\begin{pmatrix} -\frac{1}{2m_d} & \psi'_d(0+) \\ -\frac{1}{2m_n} & \psi'_n(0+) \end{pmatrix} + W \begin{pmatrix} A\psi_d(0+) \\ B\psi_n(0+) \end{pmatrix} = 0 \quad , \quad (2.7)$$

with W a symmetric, constant, 2×2 matrix.

We now explicitly limit our attention to the case where the nuclear system (${}^5\text{He}^*$) has an energy such that the dt -channel d is closed and the $n\alpha$ -channel n is open.

Introducing in the effective nuclear interaction an energy shift between the n and d channels to account for the difference in the channel thresholds one has

$$E_{\text{nuc1}} = \frac{1}{2m_n} \kappa^2 = E_{\text{shift}} + \frac{1}{2m_d} k^2 \quad (2.8)$$

Thus at the energy under consideration, κ is the wave number in the open n channel and k is the wave number in the closed d channel, both corresponding to the same energy for the ${}^5\text{He}^*$ system. Thus the wave function for the system has the form:

$$\psi = \begin{pmatrix} A e^{-\kappa r_d} \\ B \sin(\kappa r_n + \delta_n) \end{pmatrix} \quad (2.6a)$$

Introducing this into (2.7) we find that:

$$M \begin{pmatrix} A \\ B \end{pmatrix} := \begin{pmatrix} \frac{k}{2m_d} + W_{dd} & W_{nd} \sin \delta_n \\ W_{nd} & -\frac{\kappa}{2m_n} \cos \delta_n + W_{nn} \sin \delta_n \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = 0 \quad (2.7a)$$

The requirement that a non-trivial solution exist, is the condition that

$$\text{Det } M = 0 \quad , \quad (2.9a)$$

where M is the matrix above. This condition is found to be:

$$(k + 2m_d W_{dd}) (-\kappa \cot \delta_n + 2m_n W_{nn}) = 4m_n m_d (W_{nd})^2 \quad (2.9b)$$

Since according to eq (2.8) the d-channel wave numbers k is determined by the n-channel wave number κ , and since all the other parameters are constant we see that eq (2.9) expresses the phase shift δ_n as a function of the n-channel energy. Recall that this is the region where the d-channel is closed, the n-channel open.

Now let us introduce the muon into the problem.

There are very few solvable models for the hydrogen molecular ion — the prototype for the $(dt_\mu)^+$ ion — so we must be very schematic in order to achieve a solvable model. Physically the muon binds the dt -system since it has a significant probability of being between the two nuclei developing thereby an effective attraction. A reasonable facsimile of this situation would be the solvable model of a weak, long-range, attraction between the d and t nuclei as done in the finite-range model, figure 1. An even simpler model replaces this by a δ -function attraction at a distance b between the nuclei.

Thus we add to the system the attractive interaction

$$V^{dt} = -\gamma^2 \delta(r_d - b) . \quad (2.10)$$

The effect of this interaction is to replace the (dt) wave function in eq (2.6a) by

$$\psi_d = A(e^{-kr_d} + \alpha e^{+kr_d}) , \quad 0 \leq r_d < b . \quad (2.11)$$

Integrating across the singularity at $r_d = b$ yields

$$-\frac{k}{2m_d} \left[1 + \frac{e^{-kb} - \alpha e^{kb}}{e^{-kb} + \alpha e^{kb}} \right] - \gamma^2 = 0 , \quad (2.12a)$$

or,

$$k \left[1 + \frac{\alpha e^{2kb} - 1}{\alpha e^{2kb} + 1} \right] = 2m_d \gamma^2 =: \Gamma . \quad (2.12b)$$

Thus:

$$\alpha = e^{-2kb} \left(\frac{2k}{\Gamma} - 1 \right)^{-1} . \quad (2.13)$$

Let us interpret this seemingly complicated result.

The significant point is that the "muon interaction" has introduced a qualitative change in the (dt) wave function, corresponding to a reflection (the term α) from the muonic interaction potential. The interaction (given by Γ) is of order of 10^2 eV, the molecular binding energy. The "reflection coefficient" α is almost everywhere exponentially small (owing to the

"penetration factor" e^{-2kb} with b large, $b \approx 500$ fm) except when the (dt) wave number is itself very small ($\sim r$, i.e., small on a nuclear scale). The reflection is therefore a very sensitive function of the energy in the vicinity of the molecular binding energy.

The introduction of the muon interaction also changes the coupled system eq (2.7a) at nuclear distances; eq (2.9a) for $\text{Det } M = 0$ now becomes

$$\text{Det} \begin{vmatrix} k \frac{(1-\alpha)}{(1+\alpha)} - \Delta_d & \lambda \\ \lambda & \kappa \cot \delta_n - \Delta_n \end{vmatrix} = 0 \quad (2.14)$$

[Here we have re-named the parameters for simplicity of writing. In effect the short-range nuclear interaction is parametrized by $W \rightarrow \begin{pmatrix} -\Delta_d & \lambda \\ \lambda & -\Delta_n \end{pmatrix}$.]

Let us discuss the meaning of these results.

First: The reflection parameter α is a function of the energy, k , in the channel d , eq (2.13), and thus a function of the total energy E_{tot} , eq (2.8).

Second: the parameters Δ_d , Δ_n , λ are constants defined by the nuclear interaction. Both k (d -channel energy) and κ (n -channel energy) are given by E_{tot} . Thus eq (2.14) simply determines the $(n\alpha)$ phase shift δ_n of the channel n as a function of the total energy E_{tot} .

To interpret these relations further let us disconnect the channels (that is, put $\lambda = 0$). Then we see that we get (from the Hamiltonian) two separate conditions

$$k \frac{1-\alpha}{1+\alpha} = \Delta_d = -2m_d W_{dd} \quad (2.15a)$$

and

$$\kappa \cot \delta_n = \Delta_n = 2m_n W_{nn} \quad (2.15b)$$

Condition (2.15b) is obvious as it corresponds to the Fermi scattering length, but condition (2.15a) is interesting. Without the muon (that is, putting $\alpha = 0$) we get $k = \Delta_d$ — the wave number in the closed channel d is accordingly of nuclear energy scale. Now turn on the muon ($\alpha \neq 0$). Solving eq (2.15a), using eq (2.13) for α , we find:

$$k = \frac{r}{2} \{1 + e^{-rb} + 0 [(\frac{r}{\Delta_d})^2]\} \quad (2.16)$$

$$\alpha = -1 + 2 \frac{k}{\Delta_d} + \dots \quad (2.17)$$

Thus we find that k is of the order of $\Gamma/2$ — a wave-number of molecular energy scale — and the reflection parameter $\alpha = -1 + \text{small}$. Accordingly we see that there is a very strong reflection induced by the muon interaction. This is required in order to change dramatically the order of magnitude of the channel d energy. In other words, only if $\alpha = -1 + \text{small}$, can the energy of the dt-system acquire a molecular size, i.e., $k \ll W_{dd}$.

Having identified the molecular energy region let us now reconnect the two channels and hence examine eq (2.14) for the phase shift of channel n with $W_{nd} \neq 0$. Choosing the molecular energy region for k (see eq (2.16)), means that eq (2.15a) is satisfied. Accordingly, from eq (2.14), we see that $\kappa \cot \delta_n - \Delta_n$ must become larger. (Recall that $W_{nd} \neq 0$). This implies that $\delta_n \rightarrow 0$ as $k \rightarrow \Gamma/2 (1 + e^{-\Gamma b})$.

Now let us ask: at what neighboring energy do we get $\delta_n = \pi/2$? This is a tedious calculation, but the answer is remarkable simple: the difference in wave-numbers between $\delta_n = 0$ and $\delta_n = \pi/2$ is given by

$$\Delta k = \Gamma e^{-\Gamma b} \ll \Gamma . \quad (2.18)$$

In other words, the width of the molecular resonance is exponentially small compared with the molecular energy itself.

3. The Finite Range Model

Having seen the essential aspects of the interplay between the nuclear and molecular interactions in generating sharp molecular resonances we revert to the finite range model which is somewhat closer to the actual dt μ -system. Within that model we also will be in the position to discuss the diverse possible simplifications which have been employed in the treatment of the dt μ -system, and to illustrate the resulting changes in the wave function from the wave function of the "exact" treatment.

We begin with the pure nuclear case, i.e., in the absence of the muon. In our model this is mimicked by eliminating the molecular potential, i.e., by putting $h_M = 0$. This is indicated in figure 1 by the dashed line.

We first consider an energy above, but close to, the channel d threshold, i.e., $E \gtrsim 0$. Here one has two independent solutions at the same energy E . One way of generating these solutions is to begin the integration of the

Schrödinger equation at an arbitrary point $x = x_0$ using the starting conditions (in this section we will put in addition $m_n = m_d = 1$)

$$\psi^{(1)}(x_0) = 1 \quad , \quad \frac{d}{dx} \psi^{(1)}(x_0) = 0 \quad (3.1a)$$

and

$$\psi^{(2)}(x_0) = 0 \quad , \quad \frac{d}{dx} \psi^{(2)}(x_0) = 1 \quad (3.1b)$$

The resulting two solutions are sketched in figure 2. By adjusting the overall normalization two independent linear combinations of these solutions can be written, for $|x| > |a|$, as

$$\psi_d^{(1)}(x) = \cos(kx + \delta_d^{(1)}) \quad x > a \quad (3.2a)$$

$$\psi_n^{(1)}(x) = N^{(1)} \cos(\kappa x - \delta_n^{(1)}) \quad x < -a \quad (3.2b)$$

and

$$\psi_d^{(2)}(x) = \cos(kx + \delta_d^{(2)}) \quad x > a \quad (3.3a)$$

$$\psi_n^{(2)}(x) = N^{(2)} \cos(\kappa x - \delta_n^{(2)}) \quad x < -a \quad (3.3b)$$

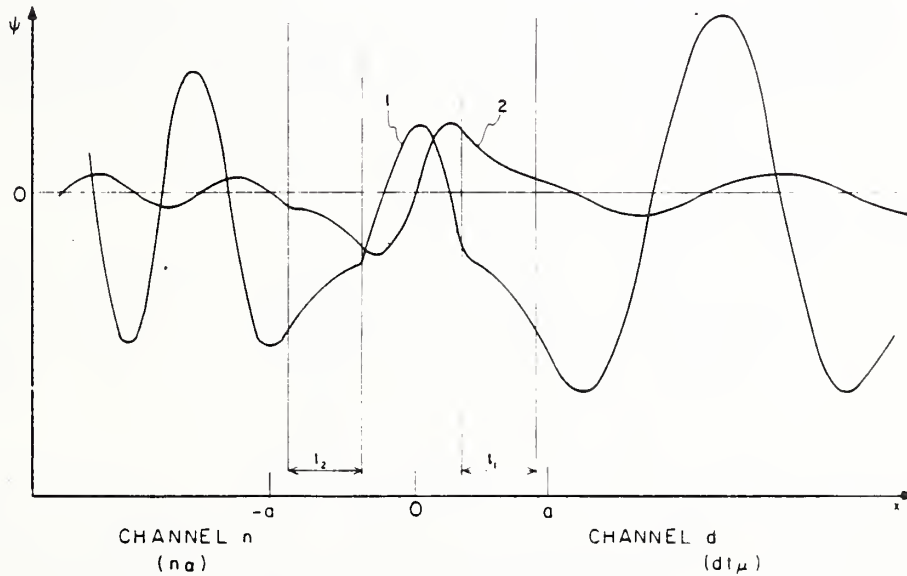


Fig. 2. The two orthogonal solutions above the channel d thresholds.

The relative normalization constants $N^{(i)}$ and the phase shifts $\delta_c^{(i)}$ depend on the choice of x_0 , but are well-defined. The starting point x_0 may be chosen to be different for the two solutions. By judicious choice of x_0 one can achieve that $\delta_d^{(1)} = \delta_n^{(1)}$ and $\delta_d^{(2)} = \delta_n^{(2)}$. The resulting solutions are called the eigenchannel solutions, they diagonalize the S-matrix of the system.

The two solutions, eq (3.2) and (3.3), (whether eigenchannel solutions or not) can be used to compute the R-Matrix. To that end we define (V denotes value and D denotes derivative, as in Wigner's original discussion):

$$V_d^{(i)} := \psi_d^{(i)}(a) = \cos(ka + \delta_d^{(i)}) \quad (3.4a)$$

$$D_d^{(i)} := \left. \frac{d\psi_d^{(i)}}{dx} \right|_{(x=a)} = -k \sin(ka + \delta_d^{(i)}) \quad (3.4b)$$

$$V_n^{(i)} := \psi_n^{(i)}(-a) = N^{(i)} \cos(\kappa a + \delta_n^{(i)}) \quad (3.5a)$$

$$D_n^{(i)} := \left. \frac{d\psi_n^{(i)}}{d(-x)} \right|_{(x=-a)} = N^{(i)} \kappa \sin(\kappa a + \delta_n^{(i)}) \quad (3.5b)$$

The minus sign in the definition of $D_n^{(i)}$ arises since in the R-matrix formalism it is defined by the derivative going away from the scattering center. Also, we should account for the fact that the reduced masses in channels d and n are different, which, however, for simplicity we shall ignore.

With the definitions (3.4), (3.5) we have:

$$\begin{pmatrix} V_d^{(i)} \\ V_n^{(i)} \end{pmatrix} = \begin{pmatrix} R_{dd} & R_{dn} \\ R_{nd} & R_{nn} \end{pmatrix} \begin{pmatrix} D_d^{(i)} \\ D_n^{(i)} \end{pmatrix}. \quad (3.6)$$

In detail, (3.6) consists of four homogeneous linear relations between the R_{cc} , and $D_c^{(i)}$, $V_c^{(i)}$. These redundant relations can be used to derive the four R-matrix elements, even though the R-matrix has only three independent parameters. The fact that $R_{dn} = R_{nd}$ can be used to check the accuracy of the solutions. As one can see immediately from the definitions (3.4), (3.5), the R-matrix depends on the choice of the "matching radius," here $x = \pm a$.

As is well known, the R-matrix elements can be written as meromorphic functions involving energy independent parameters, which can however be approximated by a few almost energy independent parameters. It has been shown, by fitting to experimental data, that the nuclear R-matrix of the ^5He -system in the neighborhood of the dt-threshold can be well represented by a background term plus a single resonance term.² Our potential model has the same characteristics. We can thus confidently use this same form to compute the R-matrix in the vicinity of $E = 0$, say within $\Delta E \approx \pm$ a few times E_M . (In our model we could check the accuracy of this representation by computing the solutions at a selection of energies).

We now are ready to consider the (purely nuclear) case $E < 0$ in more detail. Then the channel d is closed and the wave function for $x > a$ is of the form,

$$\psi_E(x) \sim e^{-Kx} \quad (3.7)$$

where we have introduced

$$K := \sqrt{2|E|} \quad . \quad (3.7a)$$

With this as "starting function" one can integrate the Schrödinger equation towards negative values of x , i.e., into the channel n, which we assume to be open at this energy. In channel n the wavefunction is given by

$$\psi_E(x) = N_n \cos(\kappa x - \delta_n) \quad , \quad x < -a \quad , \quad (3.8)$$

where again κ is the wave number in channel n corresponding to the energy E . The resulting function is sketched in figure 3. We can compute the following quantities

$$V_d(E) = \psi_E \Big|_{(x=a)} = e^{-Ka} \quad (3.9a)$$

$$D_d(E) = \frac{d\psi_E}{dx} \Big|_{(x=a)} = -K e^{-Ka} \quad (3.9b)$$

and

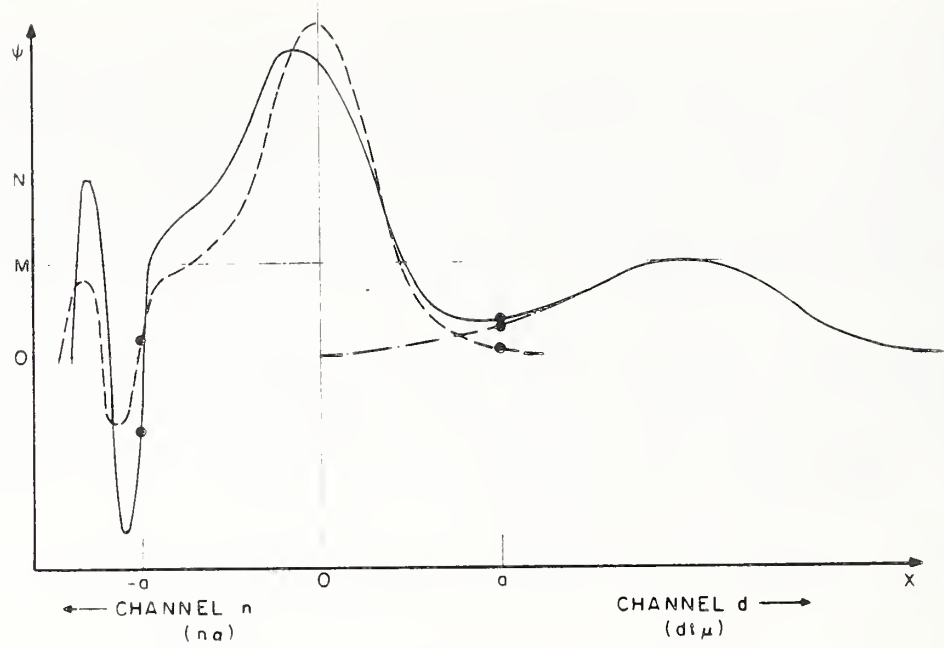


Fig. 3. Solutions for the different potentials of Fig. 1 below the channel d threshold. The little circles indicate the crossings of the channel radii $x = -a$ and $x = a$.

$$V_n(E) = \psi_E \Big|_{(x=-a)} = N_n \cos(\kappa a + \delta_n) \quad (3.10a)$$

$$D_n(E) = \frac{d\psi_E}{d(-x)} \Big|_{(x=-a)} = -\kappa N_n \sin(\kappa a + \delta_n) \quad (3.10b)$$

As before, the minus sign in (3.10b) arises since the definition of D requires differentiation outward. These quantities are again connected by the nuclear R-matrix

$$\begin{pmatrix} V_d \\ V_n \end{pmatrix} = \begin{pmatrix} R_{dd} & R_{dn} \\ R_{nd} & R_{nn} \end{pmatrix} \begin{pmatrix} D_d \\ D_n \end{pmatrix} \quad (3.11)$$

We now restore the "presence of the muon," that is, we return to the potential indicated by the full line in Fig. 1. In channel d, $x > a$, we have three regions:

$$(1) \quad x < c \quad (3.12a)$$

$$(2) \quad c < x < l \quad (3.12b)$$

$$(3) \quad x > l \quad (3.12c)$$

The wave function in these regions, for an energy $-\hbar_M < E < 0$, has the form (proceeding from the outside inward):

$$\psi_3(x) = e^{-Kx} \quad (3.13a)$$

$$\psi_2(x) = A_2 \sin(k_d x + \eta) \quad (3.13b)$$

$$\psi_1(x) = A_1 e^{-Kx} + B_1 e^{+Kx} \quad (3.13c)$$

while in channel n the form (3.8) is maintained. The procedure by which one can compute the full wave function can now be given as follows:

- (i) compute A_2 , η from the matching conditions at $x = \ell$,
- (ii) compute A_1 and B_1 from the matching conditions at $x = c$,
- (iii) use (13c) to compute V_d and D_d at $x = a$,
- (iv) use the R-matrix to compute V_n and D_n ,
- (v) compute (the non-normalized amplitude) from V_n and D_n .
- (vi) divide all amplitudes by N/N_n where N is the desired normalization constant of the continuum wave, eq (3.8).

This chain of steps can be characterized as a description of how the Hamiltonian of the system carries the consequences of the condition $\psi(x) \rightarrow 0$ for $x \rightarrow +\infty$ through the system into the matching point to the open channel n , $x = -a$, to finally determine the scattering phase shift δ . This procedure is valid for all energies E above the threshold E_T of the $n\alpha$ -channel n , as long as one has available the R-matrix at those energies. In particular, one could, in principle, find the explicit behavior of δ (the resonance associated with the quasi-bound "molecular state") by computing δ "point-by-point," at different energies, and fitting a suitable (arctan) curve to the points. This, of course, is a very unsatisfactory procedure. One would like to have to compute only the resonance position, the width of the resonance, and the background phase shift, since as we have seen in section 2 the resonance is extremely narrow, with a width $\Gamma \ll |E_M|$, where E_M is the "molecular" energy.

To illustrate this let us consider the case where the presence of the nucleus, i.e., the influence of the region $x < a$, is negligible. In that case one may use the potential indicated in figure 1 by the dash-dotted line. This potential is infinitely repulsive for $x = 0$ and constant ($V = 0$) except within the "muon well." Such a potential mimics the actual $dt\mu$ -system when neglecting the nuclear forces entirely, and implies the new boundary condition

$$\psi(x = 0) = 0 \quad . \quad (3.14)$$

With this boundary condition (3.14) and the boundary condition $\psi(+\infty) = 0$ one has a well-defined eigenvalue problem, with a real eigenenergy. The wave function in the region $x < c$ is given by (3.13c) with $E = E_M$ and

$$A_1^{(0)} = - B_1^{(0)} \quad , \quad (3.15)$$

owing to (3.14). Let us remark that the requirement given by (3.14) effectively disconnects the two channels and hence the energy in the channel d becomes discrete. For this case the R-matrix becomes diagonal; the channel coupling matrix elements vanish. This discrete state as we have seen in section 2, will actually be "embedded in the continuum," here the open $n\alpha$ -channel n , by the fact that, in our case, the off-diagonal R-matrix elements do not vanish. We will return to this complete case below.

We now compare the solutions for our three potentials at the energy E_M , at the channel radius $x = a$. We consider the logarithmic derivative,

$$L = \left. \frac{d \log \psi}{dx} \right|_{(x=a)} \quad , \quad (3.16)$$

for our solution. The "pure nuclear" solution yields ($K_M := \sqrt{2|E_M|}$)

$$L_N = - K_M < 0 \quad , \quad (3.17a)$$

the "pure molecular" solution yields

$$L_M = \frac{K_M [1 + e^{-2aK_M}]}{[1 - e^{-2aK_M}]} > 0 \quad , \quad (3.17b)$$

while the full solution yields

$$L = \frac{K_M [-A_1 e^{-aK_M} + B_1 e^{aK_M}]}{A_1 e^{-aK_M} + B_1 e^{aK_M}} \quad , \quad (3.17c)$$

where neither A_1 nor B_1 vanishes.

As to be expected, and as can be inferred from figure 3, the full solution lies in between the "pure nuclear" and the "pure molecular" solutions. Depending on the dynamics, and also on the choice of the matching radius a , L in (3.17c) can be positive or negative.

We now will discuss the response of the system for the case where the "molecular resonance" is narrow in the sense that all other parameters characterizing the system can be considered to be constant over the width of the resonance.

It will turn out that the introduction of a propagation matrix will be very useful in the discussion to follow. We thus introduce the definition

$$\begin{pmatrix} \psi_d'(a) \\ \psi_d(a) \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} \begin{pmatrix} \psi_d'(c) \\ \psi_d(c) \end{pmatrix} \quad (3.18)$$

which we will use to propagate the logarithmic derivative in the dt-channel from $x = c$ to $x = a$. We construct this matrix using the form (3.13c) of the wave function which is valid in the region $a \leq x \leq c$. Introducing the abbreviation

$$\xi = K(c - a) \quad (3.19)$$

we obtain

$$\begin{aligned} P_{11} &= \cosh \xi =: C, & P_{21} &= -\frac{1}{K} \sinh \xi =: -\frac{S}{K}, \\ P_{12} &= -K \sinh \xi = -KS, & P_{22} &= \cosh \xi = C. \end{aligned} \quad (3.20)$$

Note that $\text{Det } P = 1$.

Using these results we find

$$L := \frac{\psi_d'(x)}{\psi_d(x)} \Big|_{(x=a)} = K \frac{\lambda - \tanh \xi}{1 - \lambda \tanh \xi}, \quad (3.21)$$

where we have introduced the logarithmic derivative (divided by K) at $x = c$:

$$\lambda := \frac{1}{K} \frac{\psi_d'(x)}{\psi_d(x)} \Big|_{(x=c)}. \quad (3.22a)$$

We obtain λ from the wave function of the "molecular potential well," that is, the wave function (3.13b). To simplify the expressions we assume a strongly repulsive potential at $x > \ell$, so that we can replace (3.13a) by the condition

$$\psi_d(\ell) = 0 \quad . \quad (3.23)$$

Then we have,

$$\psi_d(x) = M \sin k(x - \ell) \quad , \quad (3.24a)$$

$$\psi'_d(x) = Mk \cos k(x - \ell) \quad , \quad (3.24b)$$

where M is the amplitude and

$$k = \sqrt{2(h_M + E)} \quad . \quad (3.25a)$$

For the case at hand the kinetic energy T is

$$0 < T = h_M + E \leq h_M \quad . \quad (3.25b)$$

This way we obtain .

$$\lambda = \frac{k}{K} \cot kt \quad . \quad (3.22b)$$

The last step is to re-write the R -matrix in the form of a propagation matrix, propagating the wave function from the channel d to the channel n (we write ψ_d for the channel d and ψ_n for the channel n)

$$\begin{pmatrix} \psi'_n \\ \psi_n \end{pmatrix} = \begin{pmatrix} \tilde{P}_{11} & \tilde{P}_{12} \\ \tilde{P}_{21} & \tilde{P}_{22} \end{pmatrix} \begin{pmatrix} \psi'_d \\ \psi_d \end{pmatrix} \quad (3.26)$$

which has the elements

$$\begin{aligned}\tilde{p}_{11} &= \frac{-R_{11}}{R_{12}}, & \tilde{p}_{22} &= \frac{R_{22}}{R_{12}} \\ \tilde{p}_{21} &= \frac{R_{21} R_{12} - R_{11} R_{22}}{R_{12}}, & \tilde{p}_{12} &= \frac{1}{R_{12}}.\end{aligned}\quad (3.27)$$

Herewith

$$L_n := \frac{\psi'_n}{\psi_n} \Big|_{(x=-a)} = \frac{\tilde{p}_{11} L + \tilde{p}_{12}}{\tilde{p}_{21} L + \tilde{p}_{22}}. \quad (3.28)$$

We can now discuss the influence of the "molecular resonance" on the open channel n . This we do in two steps. First we rewrite eq (3.21) as

$$\begin{aligned}L &= -\frac{K}{\tanh \xi} \left[1 - \frac{\coth \xi - \tanh \xi}{\coth \xi - \lambda} \right] \\ &= -\frac{K}{\tanh \xi} + \frac{K}{(\sinh \xi)^2} \frac{1}{\coth \xi - \lambda}.\end{aligned}\quad (3.21a)$$

This shows that for small penetrability, where $\coth \xi = 1 + \epsilon$ with $\epsilon \ll 1$ and $\sinh \xi \gg 1$, L is essentially constant with value $L^{(0)} = -K/\tanh \xi$ except in a very narrow region around the pole $\lambda = \coth \xi$. The width of this region is given by $\Delta \approx (\sinh \xi)^{-2} = \epsilon \ll 1$; in this region L sweeps out the values $-\infty$ to $+\infty$. Continuing now to the $n\alpha$ region, $x < -a$, one sees from (3.28) that again only over the small region around the pole of (3.21a) will the value of L_n vary from its steady value $L_n^{(0)}$, the "background" value associated with $L^{(0)}$. Evidently if $\Delta \ll h_M$ then one may forget about the energy dependence of all slowly variable parameters, including $L_n^{(0)}$.

Next we want to determine the amplitude M of the "molecular state" in terms of the amplitude of the channel n scattering state wave function, N , eq (3.10). This we can now do since we know the phase shift δ :

$$\delta_n = \arctan \left(\frac{L_n}{\kappa} \right) - \kappa a, \quad (3.29)$$

or

$$s := \sin(\kappa a + \delta) = \frac{L_n}{(\kappa^2 + L_n^2)^{\frac{1}{2}}} \quad (3.29a)$$

$$c := \cos(\kappa a + \delta) = \frac{\kappa}{(\kappa^2 + L_n^2)^{\frac{1}{2}}} \quad (3.29b)$$

and we can retrace the chain from channel n through to the "molecular" region. In terms of the inverse transformation $\tilde{Q} = \tilde{P}^{-1}$ of (3.26) we have at $x = a$

$$\begin{pmatrix} \psi'_d(a) \\ \psi_d(a) \end{pmatrix} = N \begin{pmatrix} \tilde{Q}_{11} & \tilde{Q}_{12} \\ \tilde{Q}_{21} & \tilde{Q}_{22} \end{pmatrix} \begin{pmatrix} \psi'_n \\ \psi_n \end{pmatrix}, \quad (3.30)$$

where, in terms of the R -matrix elements we have the explicit form of \tilde{Q}

$$\begin{aligned} \tilde{Q}_{11} &= \frac{-R_{22}}{R_{21}}, & \tilde{Q}_{12} &= \frac{1}{R_{21}}, \\ \tilde{Q}_{21} &= \frac{R_{12} R_{21} - R_{11} R_{22}}{R_{21}}, & \tilde{Q}_{22} &= \frac{R_{11}}{R_{21}}. \end{aligned} \quad (3.31)$$

Proceeding now to $x = c$ by means of the transformation $Q = P^{-1}$

$$\begin{aligned} Q_{11} &= C, & Q_{12} &= SK, \\ Q_{21} &= S/K, & Q_{22} &= C, \end{aligned} \quad (3.32)$$

we have

$$\psi'_c = Mk \cos k t = Q_{11} \psi'_d(a) + Q_{12} \psi_d(a) \quad (3.33a)$$

$$\psi_c = -M \sin k t = Q_{21} \psi'_d(a) + Q_{22} \psi_d(a) \quad (3.33b)$$

which, together with (3.29), (3.30) and using $\psi'_n = L_n \psi_n$ yields

$$Mk \cos kt = [Q_{11} (\tilde{Q}_{11} L_n + \tilde{Q}_{12}) + Q_{12} (\tilde{Q}_{21} L_n + \tilde{Q}_{22})] \frac{N \kappa}{\sqrt{L_n^2 + \kappa^2}} \quad (3.34a)$$

$$- Mk \sin kt = [Q_{21} (\tilde{Q}_{11} L_n + \tilde{Q}_{12}) + Q_{22} (\tilde{Q}_{21} L_n + \tilde{Q}_{22})] \frac{k N \kappa}{\sqrt{L_n^2 + \kappa^2}}. \quad (3.34b)$$

Introducing the matrix D as

$$D := Q \tilde{Q}$$

we obtain squaring and summing (3.34a) and (3.34b)

$$(Mk)^2 = [(D_{11} L_n + D_{12})^2 + k^2(D_{21} L_n + D_{22})^2] \frac{N^2 \kappa^2}{L_n^2 + \kappa^2} \quad (3.35)$$

This equation yields our desired result, i.e., the dependence of the molecular state amplitude M on the energy, which is reflected in the logarithmic derivative L at $x = a$, in view of eq (3.28).

To obtain the extrema of M^2 as a function of L we re-write (3.35) in the form

$$(Mk)^2 = \frac{\kappa^2 N^2 F(L_n^2 + F_1 L_n + F_0)}{L_n^2 + \kappa^2} \quad (3.36)$$

where

$$\begin{aligned} F &:= D_{11}^2 + k^2 D_{21}^2 \\ F_1 &:= \frac{2(D_{11}D_{12} + k^2 D_{21}D_{22})}{F} \\ F_0 &:= (D_{12}^2 + k^2 D_{22}^2)/F \end{aligned} \quad (3.37)$$

and, evaluating

$$0 = \frac{d(Mk)^2}{dE} = \frac{d(Mk)^2}{dL_n} \frac{dL_n}{dL} \frac{dL}{dE}$$

we find the condition

$$L_n^2 - \frac{2\kappa^2 - 2F_0}{F_1} L_n - \kappa^2 = 0 \quad (3.38a)$$

which yields

$$L_n = \frac{1}{F_1} [\kappa^2 - F_0 \pm \sqrt{\kappa^4 - \kappa^2(2F_0 + F_1^2) + F_0^2}] \quad (3.38b)$$

As the last point of this analysis we consider the behavior of the system far from resonance. To that end we retreat to (3.33), insert the explicit values for Q_{CC} , from (3.32), square and sum, to arrive at

$$M^2 = N^2 \frac{c^2}{(\tilde{p}_{21} + \tilde{p}_{22} L)^2} \left[\left(C + \frac{SL}{K} \right)^2 + \left(\frac{KS + CL}{k} \right)^2 \right] . \quad (3.39a)$$

Far from the resonance we have (from eq (3.21a)) that $L \rightarrow L^{(0)} = -\frac{KC}{S}$. Inserting this value for L into (3.39a) we see that M^2 simplifies to:

$$M^2 = N^2 \frac{c^2}{(\tilde{p}_{21} + \tilde{p}_{22} L)^2} \left(\frac{K}{k} \right) \frac{1}{S^2} \quad (3.39b)$$

Since far from the resonance we also have $\coth \xi = 1 + \epsilon$, with $\epsilon \ll 1$, we see that

$$\frac{1}{S^2} = \frac{1}{(\sinh \xi)^2} \sim \epsilon \ll 1 .$$

These results suffice to show that: far from resonance the amplitude M (in the muonic region) is very small compared with the amplitude N in the $n\alpha$ -channel, that is, $M^2 \approx \epsilon N^2 \ll 1$. This completes the calculation.

4. Application to dt_μ Calculation

Having derived the diverse relations fulfilled by the model systems one still needs a prescription, an algorithm, on how to perform an actual calculation. Furthermore, this calculational procedure should not be model dependent, i.e., it should be applicable to the actual case of dt_μ -fusion. Hence, we now re-write our expressions in a model-independent form. We restrict ourselves hereby describing a method which would be practicable in the case of a single (or very few) channels. The general case will be treated in Ref. 3.

Recall that the essential model lies to the right of $x = a$, Fig. 1. To wit., the expressions for the region to the left of $x = a$ are already written in terms of the R -matrix parameters, which are known from experiment. Thus we only have to discuss the dynamics of the "molecular system" to determine which features are model-dependent and which features are model-independent.

Here the essential point is that the "molecular system" exhibits a very narrow resonance in the sense that the width $\Gamma \ll \Delta$, where Δ is the distance to the next feature (beyond a smooth background) in that system; it could be

another resonance, or a threshold. (In fact, the ratio $\Gamma/\Delta \lesssim 10^{-5}$ in the actual case.) In that case the response of the system is to an extreme accuracy that of the "standard isolated resonance," and can be specified by the energy dependence of the logarithmic derivative at the matching radius. This "standard" logarithmic derivative then is in the vicinity of the resonance

$$L_S = \cot (bE - c) - d \quad (4.1)$$

where b, c, d are constants. Equation (4.1) can be written as

$$L_S = -d + \frac{1/b}{E - c/b} \quad (4.2)$$

We now can equate the standard form (4.1) with the model form (3.21a), re-written as function of the energy. To that end we expand λ around the pole

$$\lambda(E) = \lambda(E_0) - (E - E_0) \lambda_1' \quad (4.3a)$$

with

$$\lambda_1 = - \left. \frac{d\lambda}{dE} \right|_{E=E_0} > 0 \quad (4.3b)$$

and obtain

$$L = - \frac{KC}{S} + \frac{K}{\lambda_1 S^2} \frac{1}{E - E_0} \quad (3.21b)$$

which now has the standard form (4.2).

At this point one sees how one can provide for a model-independent treatment. Namely, one solves the dt_μ three-body problem with three choices of L to obtain the three solutions $E_1 = E(L_1)$, $E_2 = E(L_2)$, and $E_3 = E(L_3)$. With these values one can determine from eq (4.1a) or (4.1b) the three model-independent parameters b, c, d . Now one can use (3.28) and (3.29) to compute the continuation of the fusing state into the channel n . Finally, the normalization of the molecular state is determined by (3.30) by demanding

$$\psi_d(a) = N(\tilde{Q}_{21} L_n + \tilde{Q}_{22}) \frac{\kappa}{(\kappa^2 + L_n)^{\frac{1}{2}}} \quad (4.4)$$

where, as in (3.10), N is defined by the standard standing-wave continuum normalization condition.

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